Superconductivity in a Ferromagnetic Layered Compound

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We examine superconductivity in layered systems with large Fermi-surface splitting due to coexisting ferromagnetic layers. In particular, the hybrid ruthenate-cuprate compound $RuSr_2GdCu_2O_8$ is examined on the coexistence of the superconductivity and the ferromagnetism, which has been observed recently. We calculate critical fields of the superconductivity taking into account the Fulde-Ferrell-Larkin-Ovchinnikov state in a model with Fermi-surfaces which shapes are similar to those obtained by a band calculation. It is shown that the critical field is enhanced remarkably due to a Fermi-surface effect, and can be high enough to make the coexistence possible in a microscopic scale. We also clarify the direction of the spatial oscillation of the order parameter, which may be observed by scanning tunneling microscope experiments.

Recently, coexistence of superconductivity and ferromagnetism has been reported in the hybrid ruthenate-cuprate compounds $R_{1.4}Ce_{0.6}RuSr_2Cu_2O_{10-\delta}$ (R = Eu and Gd) and $RuSr_2GdCu_2O_8$ [1–3]. These compounds have similar crystal structures to the high-T_c cuprate superconductor $YBa_2Cu_3O_7$ except that layers of CuO chains are replaced with ruthenate layers. Experimental and theoretical studies indicate that the ruthenate layers are responsible for the ferromagnetic long range order [3,4], while the cuprate layers for the superconductivity [3].

One of the remarkable features of these compounds is that the superconducting transition occurs at a temperature well below the ferromagnetic transition temperature unlike most of the other ferromagnetic superconductors. For example, in $RuSr_2GdCu_2O_8$, the superconducting transition was observed at $T_c \sim 46$K, whereas the ferromagnetic transition at $T_M \sim 132$K [1]. Therefore, the ferromagnetic order can be regarded as a rigid back ground which is not modified very much by the appearance of the superconductivity. This picture is also supported by experimental observations [1–3].

According to the first principle calculations by Pickett *et al.* [4], magnetic fields in the cuprate layers due to the ordered spin moment in the ruthenate layers are much smaller than exchange fields mediated by electrons. The exchange fields play a role like magnetic fields which act only on the spin digrees of freedom but do not create Lorentz force. Therefore, the present system is approximately equivalent to a quasi-two-dimensional system in magnetic fields nearly parallel to the layers.

However, such Fermi-surface splitting gives rise to pair-breaking effect as well as that due to a parallel magnetic field. The exchange field in $RuSr_2GdCu_2O_8$ is very large and seems to exceed the Pauli paramagnetic limit (Chandrasekar-Clogston limit) [5]. The Pauli paramagnetic limit H_P at $T = 0$ is roughly estimated from the zero field transition temperature $T_c^{(0)}$ by a simplified formula $\mu_e H_P = 1.25\,T_c^{(0)}$, where μ_e denotes the electron magnetic moment. For $RuSr_2GdCu_2O_8$, since the exchange field exists in practice, $T_c^{(0)}$ of isolated cuprate layers is not known, but it will be appropriate to assume $T_c^{(0)} \lesssim 90$K from the transition temperature of $YBa_2Cu_3O_{7+\delta}$ at the optimum electron density. Hence we obtain $\mu_e H_P \lesssim 110$K at $T = 0$ from the above formula. On the other hand, the band calculation gives an estimation $\mu_e B_{ex} = \Delta_{ex}/2 \sim 25\text{meV}/2 \sim 107$K [4]. It is remarkable that the superconducting transition occurs at such a high temperature $T_c \approx 46$K in spite of the strong exchange field of the order of the Pauli paramagnetic limit at $T = 0$.

There are some mechanisms by which the critical field of superconductivity exceeds the Pauli limit. For example, the triplet pairing superconductivity is an important candidate. However, from their crystal structures and high transition temperatures, it is plausible that the present compounds are categorized as high-T_c cuprate superconductors and therefore the superconductivity is due to an anisotropic singlet pairing with line nodes, which is conventionally called a d-wave pairing. For the singlet pairing, possibility of an inhomogeneous superconducting state that is called a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO or LOFF) state [6,7] was discussed by Pickett *et al.* [4] as a candidate for the mechanism.

On the possibility of the FFLO state, they pointed out that there are nearly flat areas in the Fermi-surfaces in $RuSr_2GdCu_2O_8$, which favor the FFLO state. It is known that the FFLO critical field diverges at $T = 0$ in one dimensional models. However, if the Fermi-surfaces are too flat, nesting instabilities, such as those to spin density wave (SDW) and charge density wave (CDW), are favored for realistic interaction strengths. For the present compound, the nearly flat areas are not so flat that the nesting instabilities occur, but the small curvature still enhances the FFLO state [8].

It is also known that even in the absence of the flat areas, the critical field is enhanced in the two-dimensional (2D) systems in comparison to the three dimensional systems [9,8,10,11]. Further, when the Fermi-surface structure of the system satisfies a certain condition, the critical field can reach several times the Pauli limit even in the

absence of nearly flat areas [12]. Such a Fermi-surface effect can be regarded as a kind of nesting effects analogous to those for SDW and CDW [8]. The "nesting" effect was examined in details in our previous papers, where 2D tight binding models are studied as examples [11,12].

Direct evidence of the FFLO state may be obtained by scanning tunneling microscope (STM) experiments. For a comparison with experimental results, spatial structure of the order parameter should be predicted theoretically. In particular, direction of the modulation of the order parameter is important. It may appear that the modulation must be in the direction perpendicular to the flattest area of the Fermi-surface, because then the spatial variation is minimized. However, in some of 2D models, it is not perpendicular to flattest areas [11,12]. Only explicite calculations which take into account the Fermi-surface structure could clarify the direction of the modulation.

Therefore, the purposes of this paper are (1) estimation of the critical field of superconductivity including the FFLO state to examine the possibility of coexistence of singlet superconductivity and ferromagnetism in a microscopic scale, and (2) clarification of the direction of the spatial oscillation of the order parameter to compare with results of STM experiments possible in the future. We examine a tight binding model with Fermi-surfaces which shapes are similar to those of $RuSr_2GdCu_2O_8$, because the quantities that we are calculating are sensitive to the Fermi-surface structure.

Recently, the FFLO state has been studied in a tight binding model with only nearest neighbor hopping [12,13]. It was found that ratio of the FFLO critical field and the Pauli limit is small near the half filling. Zhu *et al.* have discussed that hence the coexistence of the superconductivity and the ferromagnetic order is difficult except in the vicinity of the ferromagnetic domains near the half filling [13,14]. However, some experimental results indicate coexistence in a microscopic scale and a bulk Meissner-state [1,15]. Here, we should note that the tight binding model with only nearest neighbor hopping can not reproduce the shapes of the Fermi-surfaces of $RuSr_2GdCu_2O_8$. By taking into account the realistic Fermi-surface structure, we will show below that the critical field is enhanced remarkably and thus the coexistence in a microscopic scale is possible in this compound.

First, we define the tight binding model

$$H_0 = \sum_{\mathbf{p}\sigma} \epsilon_{\mathbf{p}\sigma} c^\dagger_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma} \tag{1}$$

with a dispersion relation

$$\epsilon_{\mathbf{p}\sigma} = -2t(\cos p_x + \cos p_y) - 4t_2 \cos p_x \cos p_y - \mu + h\sigma, \tag{2}$$

where h denotes the exchange field. When we apply the present theory to type II superconductors in a magnetic field $\mathbf{B}$, h is written as $h = \mu_e|\mathbf{B}|$. We use a unit with $t = 1$ and the lattice constant $a = 1$ in this paper.

We take the value of the second nearest neighbor hopping energy $t_2 = -0.6t$, which gives shapes of the Fermi-surfaces similar to the symmetric CuO_2 barrel Fermi-surfaces obtained by Pickett *et al.* [4] at $n = 1.1$ as shown in Fig.1. Here, n is the electron number par a site.

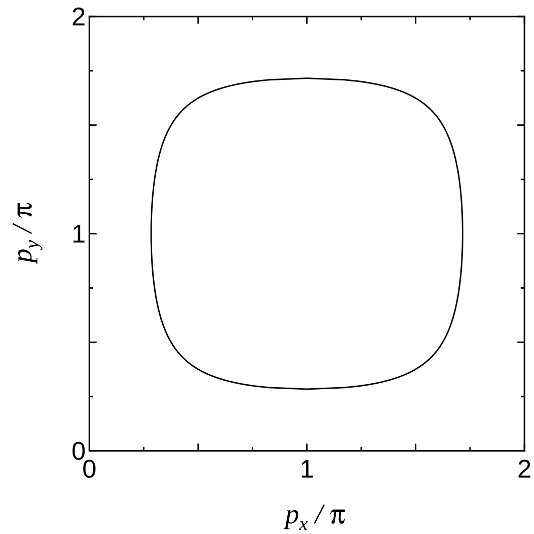

FIG. 1. Fermi-surface of the present model Hamiltonian for $t_2 = -0.6$ and $n = 1.1$.

We calculate the critical field in the ground state for $n = 0.92 \sim 2$, applying a formula developed in our previous papers [11,12]. For anisotropic pairing

$$\Delta(\hat{\mathbf{p}}, \mathbf{r}) = \Delta_\alpha \gamma_\alpha(\hat{\mathbf{p}})\, e^{i\mathbf{q}\cdot\mathbf{r}} \tag{3}$$

($\hat{\mathbf{p}} \equiv \mathbf{p}/|\mathbf{p}|$), the critical field is give by

$$h_c = \max_{\mathbf{q}} \Big[\frac{\Delta_{\alpha 0}}{2} \exp\big(-\int \frac{dp_\parallel}{2\pi} \frac{\rho^\alpha_\perp(0,p_\parallel)}{N_\alpha(0)} \log|1 - \frac{\mathbf{v}_F\cdot\mathbf{q}}{2h_c}| \big) \Big], \tag{4}$$

where $\Delta_{\alpha 0} \equiv 2\omega_D \exp(-1/g_\alpha N_\alpha(0)) \approx 1.76 k_B T_c$ and $\rho^\alpha_\perp(0,p_\parallel) \equiv \rho_\perp(0,p_\parallel)[\gamma_\alpha(\hat{\mathbf{p}})]^2$ with the momentum dependent density of states $\rho_\perp(\epsilon, p_\parallel)$. Here, $p_\parallel$ denotes the momentum component along the Fermi-surface. The pairing interaction is assumed to have a form

$$V(\mathbf{p}, \mathbf{p}') = -g_\alpha \gamma_\alpha(\hat{\mathbf{p}})\gamma_\alpha(\hat{\mathbf{p}}'). \tag{5}$$

In particular, for d-wave pairing, we use a model with

$$\gamma_d(\hat{\mathbf{p}}) \propto \cos p_x - \cos p_y, \tag{6}$$

where p_x and p_y are the momentum components on the Fermi-surface in the directions of $\hat{\mathbf{p}}$. In our previous papers, it was shown that the qualitative and semi-quantitative results are not sensitive to details of the form of $\gamma_d(\hat{\mathbf{p}})$ [11,12]. An effective density of states $N_\alpha(0)$ for anisotropic pairing is defined by

$$N_\alpha(0) \equiv N(0)\langle[\gamma_\alpha(\hat{\mathbf{p}})]^2\rangle, \tag{7}$$

with an average on the Fermi-surface

$$\langle\cdots\rangle = \int \frac{dp_\parallel}{2\pi} \frac{\rho_\perp(0,p_\parallel)}{N(0)} (\cdots)_{|\mathbf{p}| = p_F(p_\parallel)}, \tag{8}$$

where $N(0)$ is the density of states at the Fermi level. The Pauli limit $H_{\rm P}$ for anisotropic pairing is calculated by

$$\mu_e H_{\rm P} = \frac{\sqrt{\langle[\gamma_\alpha(\hat{\mathbf{p}})]^2\rangle}}{\bar{\gamma}_\alpha} \frac{\Delta_{\alpha 0}}{\sqrt{2}} \tag{9}$$

with

$$\frac{1}{\bar{\gamma}_\alpha} = \exp\Bigl(\frac{\langle[\gamma_\alpha(\hat{\mathbf{p}})]^2 \log[1/|\gamma_\alpha(\hat{\mathbf{p}})|]\rangle}{\langle[\gamma_\alpha(\hat{\mathbf{p}})]^2\rangle}\Bigr). \tag{10}$$

In the above equations, the vector $\mathbf{q}$ is the center-of-mass momentum of Cooper pairs of the FFLO state. From the symmetry of the system, there are four or eight equivalent optimum vectors ($\mathbf{q}_m$'s), depending on whether $\mathbf{q}$ is in a symmetry direction or not, respectively. Actually, arbitrary linear combination of $\exp(\mathrm{i}\mathbf{q}_m \cdot \mathbf{r})$ gives the same second order critical field, and the degeneracy is removed by the nonlinear term of the gap equation below the critical field [7,16]. However, regarding the critical field and the optimum direction of the oscillation of the order parameter near the critical field, it is sufficient to take a single $\mathbf{q}$ as in eq.(3).

Figures 2 and 3 show numerical results of the critical fields for $t_2 = -0.6$, with our previous results for $t_2 = 0$ (dotted lines) [12]. It is found that the critical fields are remarkably enhanced near the electron densities $n \approx 1.46$ and 1.20 for the s-wave and the d-wave pairing, respectively. For example, at the electron density $n = 1.1$, the ratios of the critical field to the Pauli paramagnetic limit are approximately equal to 1.66 and 3.19 for the s-wave and the d-wave pairing, respectively. These values (especially the latter) seem to be large enough to make the coexistence possible in $RuSr_2GdCu_2O_8$.

In Fig.3 for the d-wave pairing, both the critical fields for $\varphi_{\mathbf{q}} = \pi/4$ and $\varphi_{\mathbf{q}} = 0$ are shown, but the highest one is the final result of the critical field given by eq.(4). Here, $\varphi_{\mathbf{q}}$ is the angle between the optimum $\mathbf{q}$ and one of the crystal axes. It is shown by a numerical calculation that the critical fields for the other values of $\varphi_{\mathbf{q}}$ are lower than the higher one of the critical fields for $\varphi_{\mathbf{q}} = \pi/4$ and 0. Thus, the direction of the optimum wave vector $\mathbf{q}$ jumps from $\varphi_{\mathbf{q}} = \pi/4$ to $\varphi_{\mathbf{q}} = 0$ at $n \approx 1.63$. On the other hand, for the s-wave pairing, $\varphi_{\mathbf{q}} = \pi/4$ is the optimum in the whole region of the electron density. These behaviors are different from that for $t_2 = 0$, in which $\varphi_{\mathbf{q}} = 0$ [12].

For $t_2 = -0.6$, a cusp is seen in Fig.2 for the s-wave pairing, whereas it does not appear in Fig.3 for the d-wave pairing. The physical origin of the cusp at $n \approx 1.46$ is that the Fermi surfaces satisfy a certain condition there, which was explained in our previous paper for $t_2 = 0$ [12]. It is related to how the two Fermi-surfaces touch by the translation by the optimum $\mathbf{q}$. In the present case ($t_2 = -0.6$ and $n \approx 1.46$), the touch occurs in the (110) direction, but because of the nodes of the order parameter the "nesting" is not efficient for the d-wave pairing. Therefore, cusp does not appear for the d-wave pairing.

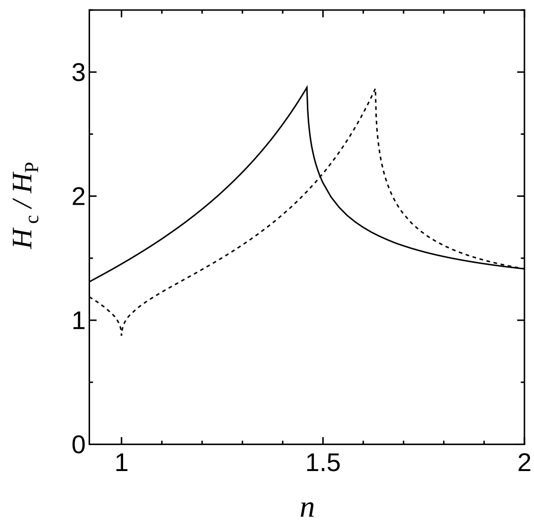

FIG. 2. Critical fields of the FFLO state of the s-wave pairing for $n = 0.92 \sim 2$ at $T = 0$. Solid and broken lines show the results for $t_2 = -0.6$ and $t_2 = 0$, respectively.

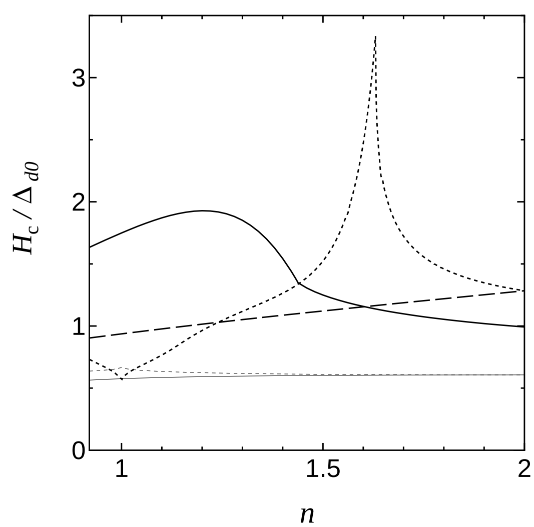

FIG. 3. Critical fields of the FFLO state of the d-wave pairing for $n = 0.92 \sim 2$ at $T = 0$. Solid and broken lines show the results for $\varphi_{\mathbf{q}} = \pi/4$ and $\varphi_{\mathbf{q}} = 0$, respectively, when $t_2 = -0.6$. The dotted line shows the result for $t_2 = 0$. Thin solid line and thin dotted line show the Pauli paramagnetic limits in the unit of Δ_{d0}, for $t_2 = -0.6$ and 0, respectively.

In spite of the absence of cusp behavior, the critical field is still very large for the d-wave pairing near the half-filling. Figure 4 shows the nesting behavior of the Fermi-surfaces at $t_2 = -0.6$ and $n = 1.1$. The direction of the optimum vector $\mathbf{q}$ is $\varphi_{\mathbf{q}} = \pi/4$, and the Fermi-surfaces touch at two points (*i.e.*, two lines in the $p_x p_y p_z$-space), $(p_x, p_y) \approx (1.113\pi, 1.713\pi)$ and $(1.713\pi, 1.113\pi)$. Since $\varphi_{\mathbf{q}} = \pi/4$ is also the direction of a node of the d-wave order parameter, it may appear that this direction is less favorable. However, in actuality the critical field

is remarkably enhanced for this "nesting" vector $\mathbf{q}$, since it gives two nesting lines which are far away from the nodes but near the flattest areas, as shown in Fig.4. Besides, they are near both the maxima of the d-wave order parameter and the van Hove singularities, which also enhance the critical field. As the electron density increases, the two nesting lines approach to the line node of the order parameter, and thus the critical field decreases.

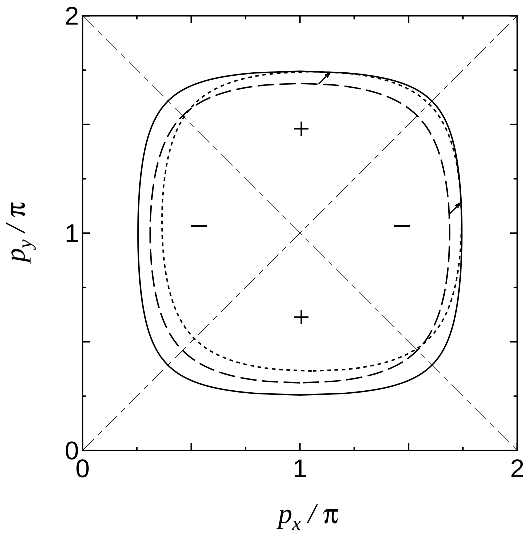

FIG. 4. Fermi-surface nesting for the FFLO state and the optimum wave vector $\mathbf{q}$ of the FFLO state at the critical field ($h_c = 1.87\Delta_{d0}$) at $n = 1.1$. Solid and broken lines show the Fermi-surfaces of the up and down spin electrons, respectively. Dotted line shows the Fermi-surface of the down spin electrons shifted by $\mathbf{q}$. Small arrows show the wave vector $\mathbf{q}$. They are placed at the momenta at which the two Fermi-surfaces touch. Dotted broken lines show the nodes of the d-wave order parameter. We use a large value of $\Delta_{d0} = 0.3t/1.87$ (*i.e.*, $h_c = 0.3t$) in order to make the displacement visible.

Since the optimum direction $\varphi_{\mathbf{q}} = \pi/4$ is in a symmetry line, there are four equivalent directions, that is, $\varphi_{\mathbf{q}} = \pm\pi/4$ and $\pm 3\pi/4$. Therefore, symmetric linear combinations such as

$$\begin{array}{lcl} \Delta(\mathbf{p},\mathbf{r}) & \propto & \cos(qx') \\ \Delta(\mathbf{p},\mathbf{r}) & \propto & \cos(qx') + \cos(qy') \end{array} \tag{11}$$

are convincing candidates, which may be observed in the present compound, where $x' = (x+y)/\sqrt{2}$ and $y' = (x-y)/\sqrt{2}$. In particular, the 2D structures such as the latter of eq.(11) are favored at high fields [16].

For the FFLO state to appear, temperature needs to be lower than the tri-critical temperature T^* of the FFLO, BCS and normal states. T^* is generally equal to about $0.56T_c^{(0)}$ in simplified models such as eq.(5). If we apply this to the present system $\mathrm{RuSr_2GdCu_2O_8}$, $T^* \gtrsim T_c \approx 46\mathrm{K}$ requires $T_c^{(0)} \gtrsim 82\mathrm{K}$. This condition for $T_c^{(0)}$ may be relaxed by taking into account a mixing of order parameters of different symmetries, which increases T^* [17].

In conclusion, the FFLO critical field of the cuprate layers is remarkably enhanced by an effect of the Fermi-surface structure. The direction of the spatial oscillation of the order parameter is in the (110) direction both for the s-wave pairing and the d-wave pairing. Although we examined only the ground state in this paper, the result $H_c/H_P \approx 3.19$ at $T = 0$ is large enough to support coexistence of the superconductivity and the ferromagnetic order in a microscopic scale in $\mathrm{RuSr_2GdCu_2O_8}$. Calculation for finite temperatures is now in progress.

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